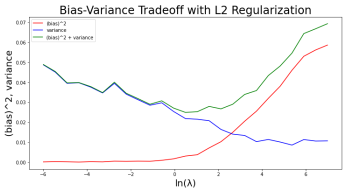
Introduction to Machine Learning

Regularization
Perspectives on Ridge Regression (Deep-Dive)



Learning goals

- Know interpretation of *L*2 regularization as row-augmentation
- Know interpretation of *L*2 regularization as minimizing risk under feature noise
- Bias-variance tradeoff for ridge regression

PERSPECTIVES ON $L2$ REGULARIZATION

We already saw two interpretations of $L2$ regularization.

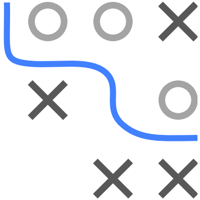
- We know that it is equivalent to a constrained optimization problem:

$$
\begin{aligned}
\hat{\theta}_{\text{ridge}} &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2 + \lambda \|\boldsymbol{\theta}\|_2^2 = (\mathbf{X}^T\mathbf{X} + \lambda \boldsymbol{I})^{-1}\mathbf{X}^T\mathbf{y} \\
&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)^2 \text{ s.t. } \|\boldsymbol{\theta}\|_2^2 \leq t
\end{aligned}
$$

- Bayesian interpretation of ridge regression: For normal likelihood contributions $\mathcal{N}(\boldsymbol{\theta}^\top \mathbf{x}^{(i)}, \sigma^2)$ and i.i.d. normal priors $\theta_j \sim \mathcal{N}(0, \tau^2)$, the resulting MAP estimate is $\hat{\theta}_{\text{ridge}}$ with $\lambda = \frac{\sigma^2}{\tau^2}$:

$$
\hat{\theta}_{\text{MAP}} = \arg\max_{\theta} \log[p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}) p(\boldsymbol{\theta})] = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2 + \frac{\sigma^2}{\tau^2} \|\boldsymbol{\theta}\|_2^2
$$

$L2$ AND ROW-AUGMENTATION

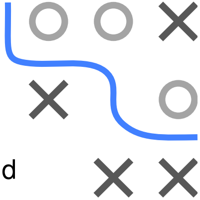


We can also recover the ridge estimator by performing least-squares on a **row-augmented** data set: Let $\tilde{\mathbf{X}} := \begin{pmatrix} \mathbf{X} \\ \sqrt{\lambda}\boldsymbol{I}_p \end{pmatrix}$ and $\tilde{\mathbf{y}} := \begin{pmatrix} \mathbf{y} \\ \mathbf{0}_p \end{pmatrix}$. Using the augmented data, the unregularized least-squares solution $\tilde{\boldsymbol{\theta}}$ can be written as

$$
\begin{aligned}
\tilde{\boldsymbol{\theta}} &= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n+p} \left(y^{\widetilde{(i)}} - \boldsymbol{\theta}^T \mathbf{x}^{\widetilde{(i)}} \right)^2 \\
&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \sum_{j=1}^{p} \left(0 - \sqrt{\lambda}\theta_j \right)^2 \\
&= \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)} \right)^2 + \lambda \|\boldsymbol{\theta}\|_2^2
\end{aligned}
$$

$\Longrightarrow \hat{\theta}_{\text{ridge}}$ is the least-squares solution $\tilde{\boldsymbol{\theta}}$ but using $\tilde{\mathbf{X}}, \tilde{\mathbf{y}}$ instead of $\mathbf{X}, \mathbf{y}$!

$L2$ AND NOISY FEATURES



Now consider perturbed features $\tilde{\mathbf{x}^{(i)}} := \mathbf{x}^{(i)} + \boldsymbol{\delta}^{(i)}$ where $\boldsymbol{\delta}^{(i)} \overset{iid}{\sim} (\mathbf{0}, \lambda \boldsymbol{I}_p)$. Note that no parametric family is assumed. We want to minimize the expected squared error taken w.r.t. the perturbations $\boldsymbol{\delta}$:

$$\mathcal{R}(\boldsymbol{\theta}) := \mathbb{E}_\delta \left[\frac{1}{n} \sum_{i=1}^{n} ((y^{(i)} - \boldsymbol{\theta}^\top \tilde{\mathbf{x}^{(i)}})^2) \right] = \mathbb{E}_\delta \left[\frac{1}{n} \sum_{i=1}^{n} ((y^{(i)} - \boldsymbol{\theta}^\top (\mathbf{x}^{(i)} + \boldsymbol{\delta}^{(i)}))^2) \right] \Big| \text{expand}$$

$$\mathcal{R}(\boldsymbol{\theta}) = \mathbb{E}_\delta \left[\frac{1}{n} \sum_{i=1}^{n} ((y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 - 2\boldsymbol{\theta}^\top \boldsymbol{\delta}^{(i)} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}) + \boldsymbol{\theta}^\top \boldsymbol{\delta}^{(i)} \boldsymbol{\delta}^{(i)\top} \boldsymbol{\theta}) \right]$$

By linearity of expectation, $\mathbb{E}_\delta[\boldsymbol{\delta}^{(i)}] = \mathbf{0}_p$ and $\mathbb{E}_\delta[\boldsymbol{\delta}^{(i)} \boldsymbol{\delta}^{(i)\top}] = \lambda \boldsymbol{I}_p$, this is

$$\begin{aligned} \mathcal{R}(\boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} ((y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 - 2\boldsymbol{\theta}^\top \mathbb{E}_\delta[\boldsymbol{\delta}^{(i)}] (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)}) + \boldsymbol{\theta}^\top \mathbb{E}_\delta[\boldsymbol{\delta}^{(i)} \boldsymbol{\delta}^{(i)\top}] \boldsymbol{\theta}) \\ &= \frac{1}{n} \sum_{i=1}^{n} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda \|\boldsymbol{\theta}\|_2^2 \end{aligned}$$

$\Longrightarrow$ Ridge regression on unperturbed features $\mathbf{x}^{(i)}$ turns out to be minimizing squared loss averaged over feature noise distribution!

BIAS-VARIANCE DECOMPOSITION FOR RIDGE

For linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\theta} + \varepsilon$ with $\mathbf{X} \in \mathbb{R}^{n \times p}$, $\varepsilon \sim (\mathbf{0}, \sigma^2 \boldsymbol{I}_n)$, bias of ridge estimator $\hat{\theta}_{\text{ridge}}$ is given by

$$
\begin{aligned}
\text{Bias}(\hat{\theta}_{\text{ridge}}) := \mathbb{E}[\hat{\theta}_{\text{ridge}} - \boldsymbol{\theta}] &= \mathbb{E}[(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^\top \boldsymbol{y}] - \boldsymbol{\theta} \\
&= \mathbb{E}[(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^\top (\boldsymbol{X}\boldsymbol{\theta} + \varepsilon)] - \boldsymbol{\theta} \\
&= (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{\theta} + (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^\top \underbrace{\mathbb{E}[\varepsilon]}_{=0} - \boldsymbol{\theta} \\
&= (\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{\theta} \\
&= \left[(\boldsymbol{X}^\top \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} - (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \right] \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{\theta}
\end{aligned}
$$

- Last expression shows bias of ridge estimator only vanishes for $\lambda = 0$, which is simply (unbiased) OLS solution
- It follows $\|\text{Bias}(\hat{\theta}_{\text{ridge}})\|_2^2 > 0$ for all $\lambda > 0$

BIAS-VARIANCE DECOMPOSITION FOR RIDGE / 2

For the variance of $\hat{\theta}_{\text{ridge}}$, we have

$$\text{Var}(\hat{\theta}_{\text{ridge}}) = \text{Var}\left((\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\mathbf{y}\right) \qquad \Big| \text{ apply } \text{Var}_u(\mathbf{A}\mathbf{u}) = \mathbf{A}\text{Var}(\mathbf{u})\mathbf{A}^\top$$

$$= (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\text{Var}(\mathbf{y})\left((\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\right)^\top$$

$$= (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\text{Var}(\varepsilon)\mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}$$

$$= (\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\sigma^2\mathbf{I}_n\mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}$$

$$= \sigma^2(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}\mathbf{X}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_p)^{-1}$$

- $\text{Var}(\hat{\theta}_{\text{ridge}})$ is strictly smaller than $\text{Var}(\hat{\theta}_{\text{OLS}}) = \sigma^2(\mathbf{X}^\top\mathbf{X})^{-1}$ for any $\lambda > 0$, meaning matrix of their difference $\text{Var}(\hat{\theta}_{\text{OLS}}) - \text{Var}(\hat{\theta}_{\text{ridge}})$ is positive definite (bit tedious derivation)
- This further means $\text{trace}\big(\text{Var}(\hat{\theta}_{\text{OLS}}) - \text{Var}(\hat{\theta}_{\text{ridge}})\big) > 0 \, \forall\lambda > 0$

BIAS-VARIANCE DECOMPOSITION FOR RIDGE / 3

With bias and variance of the ridge estimator we can decompose its mean squared error as follows:

$$\text{MSE}(\hat{\theta}_{\text{ridge}}) = \|\text{Bias}(\hat{\theta}_{\text{ridge}})\|_2^2 + \text{trace}\big(\text{Var}(\hat{\theta}_{\text{ridge}})\big)$$

Comparing MSEs of $\hat{\theta}_{\text{ridge}}$ and $\hat{\theta}_{\text{OLS}}$ and using $\text{Bias}(\hat{\theta}_{\text{OLS}}) = 0$ we find

$$\text{MSE}(\hat{\theta}_{\text{OLS}}) - \text{MSE}(\hat{\theta}_{\text{ridge}}) = \underbrace{\text{trace}\big(\text{Var}(\hat{\theta}_{\text{OLS}}) - \text{Var}(\hat{\theta}_{\text{ridge}})\big)}_{>0} - \underbrace{\|\text{Bias}(\hat{\theta}_{\text{ridge}})\|_2^2}_{>0}$$

Since both terms are positive, sign of their diff is *a priori* undetermined. ▸ Theobald 1974 and ▸ Farebrother 1976 prove there always exists some $\lambda^* > 0$ so that

$$\text{MSE}(\hat{\theta}_{\text{OLS}}) - \text{MSE}(\hat{\theta}_{\text{ridge}}) > 0$$

Important theoretical result: While Gauss-Markov guarantuees $\hat{\theta}_{\text{OLS}}$ is best linear unbiased estimator (BLUE), there are biased estimators with lower MSE.